Exact Quantum MC Methods

— without the need of a variation

1) Path Integral Monte Carlo ←
2) Diffusion (Green's function) Monte Carlo

Dimensionless Quantum Mechanics - Example → HO

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \right)\psi = E\psi$$

$V(x) = \frac{1}{2}kx^2$

$V(x) = \frac{1}{2}m\frac{k}{m}x^2$

$= \frac{1}{2}m\omega^2 x^2$

choose $x = a x^*$ ← dimensionless

↑ length scale to be choosen.

$\frac{\hbar^2}{ma^2}$ is an energy

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{a^2\partial x_*^2} + \frac{1}{2}m\omega^2 a^2 x_*^2 = E$$

divide by $\frac{\hbar^2}{ma^2}$

$$-\frac{1}{2}\frac{\partial^2}{\partial x_*^2} + \frac{1}{2}m\omega^2 a^2 \frac{ma^2}{\hbar^2}x_*^2 = E\frac{ma^2}{\hbar^2}$$

↑ choose a such that $\frac{m\omega^2 a^2 m a^2}{\hbar^2} = 1$

$m^2\omega^2 a^4 = \hbar^2$

$a^4 = \frac{\hbar^2}{m^2\omega^2}$

$a^2 = \frac{\hbar}{m\omega}$

$\boxed{a = \sqrt{\frac{\hbar}{m\omega}}}$ harmonic length

$$-\frac{1}{2}\frac{\partial^2}{\partial x_*^2} + \frac{1}{2}x_*^2 = E\frac{\cancel{m}}{\hbar^{\cancel{2}}}\frac{\cancel{\hbar}}{\cancel{m}\omega}$$

$$= \frac{E}{\hbar\omega} = E^*$$

dimensionless form ↪

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial x_*^2} + \frac{1}{2}x_*^2\right)\psi = E^*\psi$$

$E = E^*\hbar\omega$

Quantum dynamics - time-dependent Sch. Eq.

$$i\hbar\frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi$$

$$i\hbar\frac{ma^2}{\hbar^2}\frac{\partial}{\partial t}\psi = \left[-\frac{1}{2}\frac{\partial^2}{\partial x_*^2} + \frac{1}{2}x_*^2\right]\psi$$

$$i\frac{ma^2}{\hbar} = i\frac{\cancel{m}}{\cancel{\hbar}}\frac{\cancel{\hbar}}{\cancel{m}\omega}$$

$$i\frac{\partial}{\omega\partial t}\psi = (\quad)\psi$$

$$\Rightarrow \boxed{t^* = \omega t}$$

$$i\frac{\partial}{\partial t^*}\psi = (\quad)\psi$$

Apr 10-9:11 AM

Dimensionless Quantum Dynamics → remove all *

$$i\frac{\partial}{\partial t}\psi = \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2\right)\psi$$

$$= (T + V)\psi$$

Solution : $\frac{1}{\psi}\frac{\partial\psi}{\partial t} = -i\,(T+V)\,\cancel{\psi}$

$$\frac{\partial}{\partial t}\ln\psi = -i\,(T+V)$$

$$\ln\psi = -it\,(T+V) + c$$

$$\boxed{\psi(t,x) = e^{-it(T+V)}\,\psi(0,x)}$$

next week

The case of imaginary time-propagation. $t = -i\tau$

$$\psi(\tau,x) = e^{-\tau(T+V)}\,\psi(0,x)$$

$$= e^{-\tau H}\sum_{n=0}^{\infty} C_n\psi_n(x) \qquad H\psi_n = E_n\psi_n$$

$$= \sum_{n=0}^{\infty} C_n\, e^{-\tau H}\psi_n(x)$$

$$[1 - \tau H + \tfrac{1}{2}\tau^2H^2 \cdots]\psi_n$$

$$= \sum_{n=0}^{\infty} C_n e^{-\tau E_n}\psi_n$$

$\lim_{\tau\to\infty}\psi(\tau,x)$

$\longrightarrow C_0 e^{-\tau E_0}\psi_0(x) + C_1 e^{-\tau E_1}\psi_1(x)$

$\longrightarrow C_0 e^{-\tau E_0}\psi_0(x)$

$\tau\to\infty$ gives the ground state of H.

idea of Diffusion Monte Carlo.

The path-integral MC.

Propagator or Green's function of the Sch. Eq.

$$G(x';x;\tau) = \langle x' | e^{-\tau H} | x \rangle$$

density matrix

$$= \sum_n \langle x' | e^{-\tau H} | \psi_n \rangle \langle \psi_n | x \rangle$$

$$= \sum_n \langle x' | \psi_n \rangle e^{-\tau E_n} \langle \psi_n | x \rangle$$

$$= \sum_n \psi_n^*(x') \psi_n(x) e^{-\tau E_n}$$

$$\lim_{x' \to x} \lim_{\tau \to \infty} G(x';x,\tau) \longrightarrow \psi_0^*(x) \psi_0(x) e^{-\tau E_0} + \cdots$$

to solve $$= |\psi(x)|^2 e^{-\tau E_0} + \cdots$$

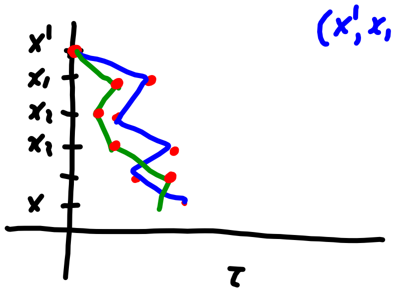
for the exact g.s. property $\rightarrow$ evolve $G(x';x,\tau)$ to large τ.

$$G(x',x;\tau) = \langle x'|\, e^{-\tau H}\, |x\rangle \qquad \tau = n\,\Delta\tau$$

$$= \langle x'|\, e^{-\Delta\tau H}\, e^{-\Delta\tau H}\, e^{-\Delta\tau H} \dots |x\rangle$$

$$= \int dx_1\, dx_2 \quad \langle x'|\, e^{-\Delta\tau H} |x_1\rangle\langle x_1|\, e^{-\Delta\tau H} |x_2\rangle\langle x_2|\, e^{-\Delta\tau H} |x\rangle$$

$$= \int dx_1\, dx_2 \quad G(x',x_1,\Delta\tau)\, G(x_1,x_2,\Delta\tau)\, G(x_2,x,\Delta\tau)$$

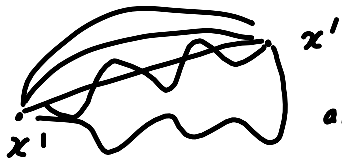


$(x', x_1, x_2 \dots x)$

integration over $x_1 \dots x_n$

$\Rightarrow$ Sum of all paths

path Integral



all path.

Approximate $\langle x'|e^{-\Delta\tau H}|x\rangle \sim \langle x'|\, e^{-\Delta\tau T}\, e^{-\Delta\tau V}\, |x\rangle$

$$\sim \langle x'|\, e^{-\frac{1}{2}\Delta\tau V}\, e^{-\Delta\tau T}\, e^{-\frac{1}{2}\Delta\tau V} |x'\rangle$$

Short time propagator:

$$G(x,x';\Delta\tau) = \langle x| e^{-\frac{1}{2}\Delta\tau V} e^{-\Delta\tau T} e^{-\frac{1}{2}\Delta\tau V} |x'\rangle$$

$$= e^{-\frac{1}{2}\Delta\tau V(x)} \langle x| e^{-\Delta\tau T} |x'\rangle e^{-\frac{1}{2}\Delta\tau V(x')}$$

$$\langle x| e^{-\Delta\tau\left(-\frac{1}{2}\nabla^2\right)} |x'\rangle = \langle x| e^{-\Delta\tau \frac{1}{2}p^2} |x'\rangle$$

$$\langle x| e^{-\Delta\tau T} |x'\rangle = \frac{1}{\sqrt{2\pi\Delta\tau}} e^{-\frac{1}{2\Delta\tau}(x-x')^2}$$

$$= \int \frac{dp}{2\pi} \langle x| e^{-\Delta\tau\frac{1}{2}p^2} |p\rangle\langle p|x'\rangle$$

$$= \int \frac{dp}{2\pi} \langle x|p\rangle \langle p|x'\rangle e^{-\Delta\tau \frac{1}{2}p^2}$$

$$e^{-ipx} \quad e^{ipx'} \qquad \frac{e^{ipx'}}{\sqrt{2\pi}}$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{-\frac{1}{2}\Delta\tau p^2} e^{ip(x'-x)} \qquad g = \frac{i}{\Delta\tau}(x'-x)$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{-\frac{1}{2}\Delta\tau\left(p^2 - \frac{2}{\Delta\tau} ip(x'-x)\right)}$$

$$(p^2 - 2gp + g^2 - g^2)$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{-\frac{1}{2}\Delta\tau(p-g)^2} e^{-\frac{1}{2}\Delta\tau \frac{1}{\Delta\tau^2}(x'-x)^2}$$

$$= \int_{-\infty}^{\infty} \frac{dp'}{2\pi} e^{-\frac{1}{2}\Delta\tau p'^2} \qquad \int dx\, e^{-\frac{1}{2\Delta t}x^2} = \sqrt{2\pi\Delta t}$$

$$e^{-\frac{1}{2(1/\Delta\tau)}p'^2}$$

$$= \frac{1}{2\pi}\sqrt{2\pi\frac{1}{\Delta t}} = \frac{1}{\sqrt{2\pi\Delta t}} \quad e^{-\frac{1}{2\Delta\tau}(x'-x)^2}$$

The second-order (primitive)

$$G_2(x,x';\Delta\tau) = \frac{1}{\sqrt{2\pi\Delta\tau}} e^{-\frac{1}{2\Delta\tau}(x-x')^2} e^{-\Delta\tau\frac{1}{2}(V(x)+V(x'))}$$

$$= e^{-\frac{1}{2}\ln(2\pi\Delta\tau) - \cdots \quad ''}$$

$$= e^{-S_2(x,x';\Delta\tau)}$$

$$S_2 = \frac{1}{2}\ln(2\pi\Delta\tau) + \frac{1}{2\Delta\tau}(x-x')^2 + \Delta\tau\frac{1}{2}(V(x)+V(x'))$$

$$G(x_1\,x_2;\Delta\tau)\,G(x_2x_3;\Delta\tau)\cdots$$
$$= e^{-[S_2(x_1x_2\,\Delta\tau)+S_2(x_2x_3\,\Delta\tau)+\cdots]}$$

$$Z = \int dx_1dx_2\cdots dx_n\; G(x_1x_2)\,G(x_2x_3)\cdots G(x_{n-1},x_n)\,G(x_n,x_1)$$

n-bead path Integral. $\tau = n\Delta\tau$

for large τ, need larger n-bead PI

Compute the ground state energy

$$\langle E_L\rangle = \frac{\int dx_1\cdots dx_n\; H_1 G(x_1x_2)\cdots}{\int dx\cdots\; G(x_1x_2\cdots)}$$

$$= \frac{\int dx_1\cdots dx_n\;\frac{H_1G(x_1x_2)}{G(x_1,x_2)}G(x_1,x_2)\cdots}{\int dx_1\cdots G\cdots}$$

$$= \frac{\int dx_1\cdots dx_n\;\underbrace{\frac{H_1G(x_1x_2)}{G(x_1,x_2)}}_{E_L(x_1x_2)}\,\mathcal{R}(x_1\cdots x_n)}{\int dx\cdots\;\mathcal{R}(x_1\cdots x_n)}$$

$$E_L = \left\langle \frac{1}{n}\sum_{i=1}^{n} E_L(x_i,x_{i+1})\right\rangle \qquad n+1=1$$

This calculation corresponds to

$$G(x,x';\Delta\tau) = \langle x| e^{-\Delta\tau H}|x'\rangle$$

exact

$$\sum \psi_n^*(x)\psi_n(x')$$

$$E = \lim_{x'\to x} \frac{\int dx\, H G(x,x';\Delta\tau)}{\int dx\, G(x,x,\Delta\tau)} = \int dx\, H \sum_n \psi_n(x)\psi_n(x') e^{-\Delta\tau E_n}$$

$$= \sum_n \int dx\, \psi_n^2(x) E_n e^{-\Delta\tau E_n}$$

$$= \frac{\sum_n E_n e^{-\Delta\tau E_n}}{\sum_n e^{-\Delta\tau E_n}} = \frac{-\frac{\partial}{\partial\Delta\tau}\sum_n e^{-\Delta\tau E_n}}{\underbrace{\sum_n e^{-\Delta\tau E_n}}_{= Z}} = \boxed{-\frac{\partial}{\partial\Delta\tau}\ln Z = F(\Delta\tau)}$$

$$F(\Delta\tau) \underset{\Delta\tau\to\infty}{\to} E_0$$

for HO

$$Z = \sum_{n=0}^{\infty} e^{-\Delta\tau(n+\frac{1}{2})} = e^{-\Delta\tau\frac{1}{2}} \sum_{n=0} e^{-\Delta\tau n} = e^{-\Delta\tau\frac{1}{2}} \frac{1}{1-e^{-\Delta\tau}}$$

$1+x+x^2+\ldots$

$$\ln Z = -\Delta\tau\frac{1}{2} - \ln(1-e^{-\Delta\tau})$$

$$-\frac{\partial \ln Z}{\partial\tau} = \frac{1}{2} + \frac{e^{-\tau}}{1-e^{-\tau}}$$